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We Claim:

1. A parallel, combinatorial method for the discovery and optimization of novel catalysts for chemical transformations, comprising:

(a) chemically synthesizing a variegated library of potential catalysts; and

(b) screening the library of potential catalysts to identify those members that catalyze the transformation of interest.

2. The method of claim 1, wherein the potential catalysts comprise a natural or unnatural amino acid.

3. The method of claim 1, wherein the library comprises a catalyst that catalyzes a stereoselective reaction.

4. The method of claim 1, wherein the library comprises a catalyst that catalyzes a chemoselective and/or regioselective reaction.

5. The method of claim 1, wherein the potential catalysts comprise a cyclic moiety selected from the group consisting of acridarsine, acridine, anthracene, arsindole, arsinoline, azepane, benzene, carbazole, carboline, chromene, cinnoline, furan, furazan, hexahydropyridazine, hexahydropyrimidine, imidazole, indane, indazole, indole, indolizine, isoarsindole, isobenzofuran, isochromene, isoindole, isophosphindole, isophosphinoline, isoquinoline, isorasinoline, isothiazole, isoxazole, morpholine, naphthalene, naphthyridine, oxazole, oxolane, perimidine, phenanthrene, phenanthridine, phenanthroline, phenarsazine, phenazine, phenomercurazine, phenomercurin, phenophosphazine, phenoselenazine, phenotellurazine, phenothiarsine, phenoxantimonin, phenoxaphosphine, phenoxarsine, phenoxaselenin, phenoxatellurin, phenothiazine, phenoxathiin, phenoxazine, phosphanthene, phosphindole, phosphinoline, phthalazine, piperazine, piperazine, piperidine, piperidine, pteridine, purine, pyran, pyrazine, pyrazole, pyridazine, pyridine, pyrimidine, pyrrolidine, pyrrolidine, pyrrolizine, quinazoline, quinoline, quinolizine, quinoxaline, selenanthrene, selenophene, tellurophene, tetrahydrofuran, tetrahydrothiophene, thianthrene, thiazole, thiolane, thiophene and xanthene.

6. The method of claim 1, wherein the potential catalysts comprise a bicyclo[x.y.z]alkane, where x, y, and z are each independently integers greater than or equal to zero.

7. The method of claim 1, wherein the potential catalysts comprise an asymmetric center.

8. The method of claim 1, wherein the library of potential catalysts comprises a catalyst that is not superimposable on its mirror image.

9. The method of claim 1, wherein the library comprises at least one hundred potential catalysts.

10. The method of claim 9, wherein the library comprises at least one thousand potential catalysts.

11. The method of claim 10, wherein the library comprises at least ten thousand potential catalysts.

12. The method of claim 1, wherein the potential catalysts comprise a saccharide or oligosaccharide.

13. The method of claim 12, wherein the saccharide, or oligosaccharide, consists of pentose sugars, hexose sugars, pentose azasugars, and/or hexose azasugars.

14. The method of any of claims 1-13, wherein the library is synthesized on a solid support.

15. The method of any of claims 1-13, wherein the library is synthesized in solution.

16. The method of claim 1, wherein a selected catalyst is used as the lead structure for a second library of potential catalysts; said second library of potential catalysts is screened to identify those members that catalyze the transformation of interest; at least one of the members of the second library being an improved catalyst for the transformation of interest relative to the catalyst from the first library.

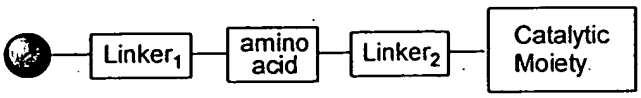
17. The method of claim 16, wherein the described process is reiterated between one and ten additional times to provide at least one improved catalyst for the transformation of interest.

18. The method of claims 1, 16 or 17, wherein a selected catalyst catalyzes a transformation selected from the set comprising kinetic resolutions, regioselective reactions, chemoselective reactions, diastereoselective reactions, stereoselective reactions, functional group interconversions, hydrogenations, oxidations, reductions, resolutions of racemic mixtures, cycloadditions, sigmatropic rearrangements, electrocyclic reactions, ring-openings, carbonyl additions, carbonyl reductions, olefin additions, olefin reductions, imine additions, imine reductions, olefin epoxidations, olefin aziridinations, carbon-carbon bond formations, carbon-heteroatom bond formations, and heteroatom-heteroatom bond formations.

19. The method of claim 1, 16, or 17, wherein the catalysts are selected based on the observation of a detectable event.

20. The method of claim 19, wherein the detectable event is a member of the set comprising the evolution of a gas, the emission of a photon, and the formation of a precipitate.

21. A library of potential catalysts, and the individual members thereof, having the following general structure:



wherein

the sphere represents a solid support;

$Linker_1$ and $Linker_2$ are independently selected from the group consisting of difunctional molecules with or without sidechains and/or stereocenters;

amino acid represents a natural or unnatural amino acid; and

the catalytic moiety is selected from the set comprising the catalytically-active portions of known catalysts.

22. The library and individual catalysts of claim 21, wherein

$Linker_1$ and $Linker_2$ are independently selected from the set comprising diamines, diols, amino alcohols, and diacids; and

the catalytic moiety is selected from the set comprising salenates, porphyrins, Schiff base-containing moieties, diketopiperazines, oligoamines, oligoalcohols, amino alcohols, oligopeptides, and oligonucleotides.

23. The library and individual catalysts of claim 22, wherein the catalytic moiety is mono-, di-, tri-, or tetra-dentate with respect to a substrate.

24. The library of claims 21, 22 or 23, wherein the library comprises at least one hundred potential catalysts.

25. The library of claims 21, 22 or 23, wherein the library comprises at least one thousand potential catalysts.

26. The library of claims 21, 22 or 23, wherein the library comprises at least ten thousand potential catalysts.

27. The library and individual catalysts of claims 21, 22 or 23, wherein a selected catalyst is used as the lead structure for a second library of potential catalysts; said second library of potential catalysts is screened to identify those members that catalyze the transformation of interest; at least one of the members of the second library being an improved catalyst for the transformation of interest relative to the catalyst from the first library.

28. The library and individual catalysts of claim 27, wherein the described process is reiterated between one and ten additional times to provide at least one improved catalyst for the transformation of interest.

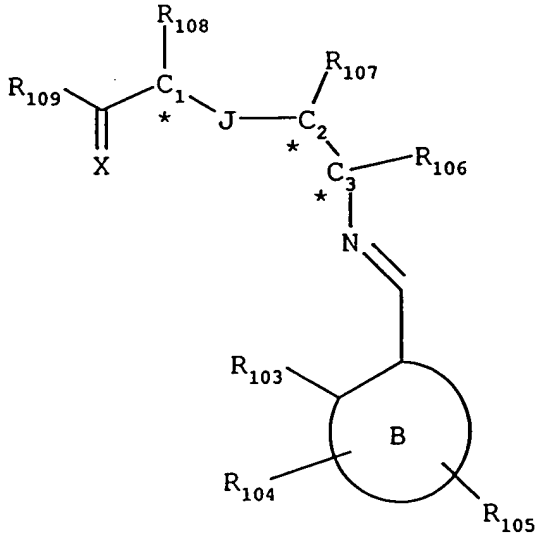
29. The method of claims 27 or 28, wherein a selected catalyst catalyzes a transformation selected from the set comprising kinetic resolutions, regioselective reactions, chemoselective reactions, diastereoselective reactions, stereoselective reactions, functional group interconversions, hydrogenations, oxidations, reductions, resolutions of racemic mixtures, cycloadditions, sigmatropic rearrangements, electrocyclic reactions, ring-openings, carbonyl additions, carbonyl reductions, olefin additions, olefin reductions, imine additions, imine reductions, olefin epoxidations, olefin aziridinations, carbon-carbon bond formations, carbon-heteroatom bond formations, and heteroatom-heteroatom bond formations.

30. The method of claims 27 or 28, wherein the catalysts are selected based on the observation of a detectable event.

31. The method of claim 30, wherein the detectable event is a member of the set comprising the evolution of a gas, the emission of a photon, and the formation of a precipitate.

32. A parallel, combinatorial method for the discovery and optimization of catalysts for a transformation from the set comprising the Strecker reaction, the aldol addition, the aldol condensation, the Michael addition, the Claisen rearrangement, the Cope rearrangement, the dihydroxylation of olefins, the epoxidation of olefins, the aziridination of olefins, the Darzen's condensation, the Diels-Alder reaction, the hetero-Diels-Alder reaction, the ene reaction, the hetero-ene reaction, the Wittig rearrangement, the Nazarov cyclization, the asymmetric addition of Grignard reagents to carbon-heteroatom π-bonds, the asymmetric addition of organolithium reagents to carbon-heteroatom π-bonds, the asymmetric Robinson annulation, and the Simmons-Smith reaction.

33. A catalyst represented by the following general structure:



wherein

B represents a monocyclic or polycyclic group;

C_1, C_2 and C_3 each represent chiral carbon atoms;

X represents O, S or NH;

J represents a linker group including at least one functional group capable of acting as a hydrogen bond donor;

R_{103} represents either a hydrogen bond donor, a Lewis basic group, or a group with both characteristics;

R_{104} represents a sterically bulky, aliphatic or cycloaliphatic substituent of up to 20 carbons (preferably 2-10);

R_{105} is absent, or represents one or more additional substituents of B selected from the group consisting of alkyl, alkenyl, alkynyl, acyl, thioacyl, alkylthio, imine, amide, phosphoryl, phosphonate, phosphine, carbonyl, carboxyl, carboxamide, anhydride, silyl, thioalkyl, alkylsulfonyl, arylsulfonyl, selenoalkyl, ketone, aldehyde, ester, heteroalkyl, amidine, acetal, ketal, aryl, heteroaryl, aziridine, carbamate, epoxide, hydroxamic acid, imide, oxime, sulfonamide, thioamide, thiocarbamate, urea, thiourea, or $-(CH_2)_m-R_{80}$; and

R_{106} and R_{107} each independently represent alkyl, alkenyl, alkynyl, acyl, thioacyl, alkylthio, imine, amide, phosphoryl, phosphonate, phosphine, carbonyl, carboxyl, carboxamide, anhydride, silyl, thioalkyl, alkylsulfonyl, arylsulfonyl, selenoalkyl, ketone, aldehyde, ester, heteroalkyl, amidine, acetal, ketal, aryl, heteroaryl, aziridine, carbamate, epoxide, hydroxamic acid, imide, oxime, sulfonamide, thioamide, thiocarbamate, urea, thiourea, or $-(CH_2)_m-R_{80}$, or

R_{106} and R_{107} taken together with C_2 and C_3 form a ring having from 4 to 8 atoms in the ring;

R_{108} and R_{109} each independently represent an alkyl, represent alkyl, alkenyl, alkynyl, acyl, thioacyl, alkylthio, imine, amide, phosphoryl, phosphonate, phosphine, carbonyl, carboxyl, carboxamide, anhydride, silyl, thioalkyl, alkylsulfonyl, arylsulfonyl, selenoalkyl, ketone, aldehyde, ester, heteroalkyl, amidine, acetal, ketal, aryl, heteroaryl, aziridine, carbamate, epoxide, hydroxamic acid, imide, oxime, sulfonamide, thioamide, thiocarbamate, urea, thiourea, or $-(CH_2)_m-R_{80}$, with the proviso that R_{108} and $(C(X)R_{109})$ are not identical (this proviso is implied by the aforementioned chirality of C_1);

R_{80} represents an unsubstituted or substituted aryl, a cycloalkyl, a cycloalkenyl, a heterocycle, or a polycycle; and

m is an integer in the range 0 to 8 inclusive.

34. A catalyst according to claim 33, wherein X is S or O.

35. A catalyst according to claim 33, wherein R_{103} is $-NH_2$, -OH, or -SH, or a lower alkyl group substituted thereby.

36. A catalyst according to claim 33, wherein R_{104} is attached to B at a position both *ortho* to R_{103}, and *meta* to the imine substituent on B.

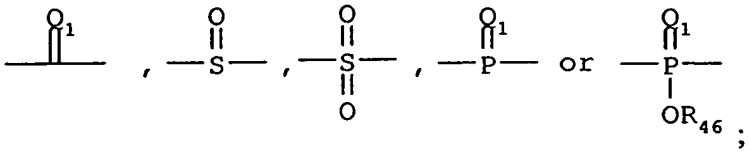
37. A catalyst according to claim 33, wherein R_{104} is a lower alkyl or alkoxyl group.

38. A catalyst according to claim 33, wherein R_{106} and R_{107} are C_3-C_8 alkyl groups, or, together with C_2 and C_3 form a ring having from 4 to 8 atoms in the ring.

39. A catalyst according to claim 33, wherein

J is represented by -NH-Y-NH-;

Y is selected from the group consisting of



;

Q_1 represents S or O; and

R_{46} represents hydrogen, a lower alkyl or an aryl.

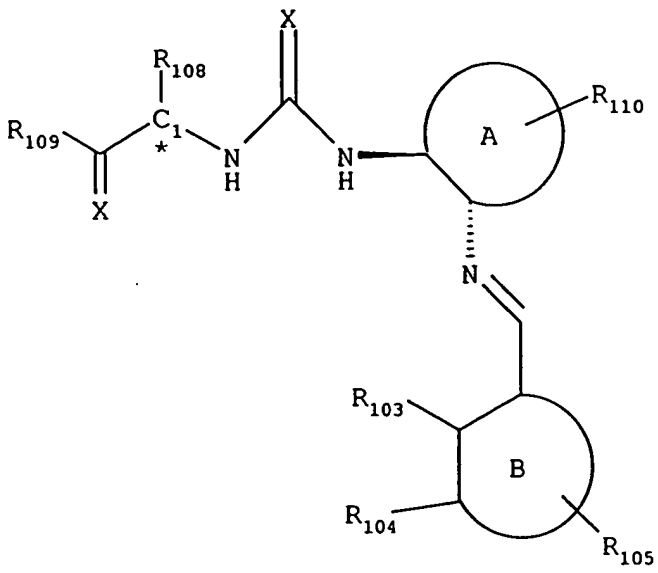
40. A catalyst according to claim 39, wherein Y is $-C(=Q_1)-$; and Q_1 is O or S.

41. A catalyst according to claim 33, wherein R_{108} represents an alkyl, heteroalkyl, aryl or heteroaryl group.

42. A catalyst according to claim 33, 39, or 40, wherein R_{108} represents a side-chain of a naturally occurring α-amino acid or analog thereof.

43. A catalyst according to claim 42, wherein R_{109} represents an amino group.

44. A catalyst represented by the following general structure:



wherein

A represents a monocyclic or polycyclic group;

B represents a monocyclic or polycyclic group;

C_1 represents a chiral carbon atom;

X represents O, S or NH;

R_{103} represents either a hydrogen bond donor, a Lewis basic group, or a group with both characteristics;

R_{104} represents a sterically bulky, aliphatic or cycloaliphatic substituent of up to 20 carbons;

R_{105} is absent, or represents one or more additional substituents of B selected from the group consisting of alkyl, alkenyl, alkynyl, acyl, thioacyl, alkylthio, imine, amide, phosphoryl, phosphonate, phosphine, carbonyl, carboxyl, carboxamide, anhydride, silyl, thioalkyl, alkylsulfonyl, arylsulfonyl, selenoalkyl, ketone, aldehyde, ester, heteroalkyl, amidine, acetal, ketal, aryl, heteroaryl, aziridine, carbamate, epoxide, hydroxamic acid, imide, oxime, sulfonamide, thioamide, thiocarbamate, urea, thiourea, or $-(CH_2)_m-R_{80}$; and

R_{108} and R_{109} each independently represent an alkyl, represent alkyl, alkenyl, alkynyl, acyl, thioacyl, alkylthio, imine, amide, phosphoryl, phosphonate, phosphine, carbonyl, carboxyl, carboxamide, anhydride, silyl, thioalkyl, alkylsulfonyl, arylsulfonyl, selenoalkyl, ketone, aldehyde, ester, heteroalkyl, amidine, acetal, ketal, aryl, heteroaryl, aziridine, carbamate, epoxide, hydroxamic acid, imide, oxime, sulfonamide, thioamide, thiocarbamate, urea, thiourea, or $-(CH_2)_m-R_{80}$, with the proviso that R_{108} and $(C(X)R_{109})$ are not identical (this proviso is implied by the aforementioned chirality of C_1);

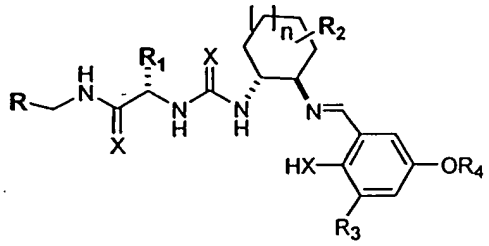
R_{110} is absent, or represents one or more additional substituents of A selected from the group consisting of alkyl, alkenyl, alkynyl, acyl, thioacyl, alkylthio, imine, amide, phosphoryl, phosphonate, phosphine, carbonyl, carboxyl, carboxamide, anhydride, silyl, thioalkyl, alkylsulfonyl, arylsulfonyl, selenoalkyl, ketone, aldehyde, ester, heteroalkyl, amidine, acetal, ketal, aryl, heteroaryl, aziridine, carbamate, epoxide, hydroxamic acid, imide, oxime, sulfonamide, thioamide, thiocarbamate, urea, thiourea, or $-(CH_2)_m-R_{80}$.

R_{80} represents an unsubstituted or substituted aryl, a cycloalkyl, a cycloalkenyl, a heterocycle, or a polycycle; and

m is an integer in the range 0 to 8 inclusive.

45. A catalyst according to claim 44, wherein A is a cycloalkyl having 5, 6 or 7 carbons in the ring structure.

46. A catalyst represented by the following general formula:



wherein

X represents, independently for each occurrence, O, S, or NR;

R, R_1, R_2, and R_3 represent, independently for each occurrence, H, alkyl, aryl, heteroalkyl, or heteroaryl;

R_4 represents H, alkyl, heteroalkyl, aryl, heteroaryl, formyl, or acyl;

R_2 is absent or occurs no more than 4 times; and

n is an integer selected from the range 0 to 2 inclusive.

47. A catalyst according to claim 46, wherein

X represents, independently for each occurrence, O or S;

R, R_1, R_2, and R_3 represent, independently for each occurrence, H, alkyl, aryl, heteroalkyl, or heteroaryl;

R_4 represents alkyl, heteroalkyl, aryl, or heteroaryl;

R_2 is absent; and

n is an integer selected from the range 0 to 2 inclusive.

48. A catalyst according to claim 47, wherein

X represents, independently for each occurrence, O or S;

R, R_1, R_2, and R_3 represent, independently for each occurrence, H, alkyl, aryl, heteroalkyl, or heteroaryl;

R_4 represents formyl or acyl;

R_2 is absent; and

n is an integer selected from the range 0 to 2 inclusive.

49. A catalyst according to claim 33, 44, or 46, wherein said catalyst catalyzes an enantioselective or diastereoselective transformation that produces a product with an enantiomeric or diastereomeric excess, respectively, of at least 75%.

50. A catalyst according to claim 33, 44, or 46, wherein said catalyst catalyzes an enantioselective or diastereoselective transformation that produces a product with an enantiomeric or diastereomeric excess, respectively, of at least 80%.

51. A catalyst according to claim 33, 44, or 46, wherein said catalyst catalyzes an enantioselective or diastereoselective transformation that produces a product with an enantiomeric or diastereomeric excess, respectively, of at least 85%.

52. A catalyst according to claim 33, 44, or 46, wherein said catalyst catalyzes an enantioselective or diastereoselective transformation that produces a product with an enantiomeric or diastereomeric excess, respectively, of at least 90%.

53. A catalyst according to claim 33, 44, or 46, wherein said catalyst catalyzes an enantioselective or diastereoselective transformation that produces a product with an enantiomeric or diastereomeric excess, respectively, of at least 95%.

54. A catalyst according to claim 33, 44, or 46, wherein said catalyst catalyzes an enantioselective or diastereoselective transformation that produces a product with an enantiomeric or diastereomeric excess, respectively, of at least 98%.